

Up Close on LDRD

A monthly insert on special topics at Lawrence Livermore National Laboratory. This month: Laboratory Directed Research & Development. • • • June 2003

Focus On LDRD

—Rokaya Al-Ayat
Associate Deputy Director of S&T



Funding innovative science gives Lab R&D vitality

Think of the most innovative science and engineering programs at the Lab and chances are those projects have an LDRD pedigree. The myriad achievements described in this *Newsline* insert are but a small sample of the award-winning, cutting-edge research and development (R&D) funded by the LDRD Program. Selecting these samples proved to be a challenge.

The name of our program reveals the key to this success. Laboratory Directed Research and Development means that we, as a Laboratory, can use up to six percent of our budget to invest in innovative science and engineering projects that ensure the scientific and technical vitality of the Laboratory and enhance our ability to meet the challenges of our evolving missions.

The ability to invest in the Laboratory's future by funding innovative, high-risk, high-potential-payoff R&D in pursuit of Laboratory missions gives us independence, flexibility, and the technical vitality. These investments help attract and engage our most talented researchers and foster collaborations with universities, other laboratories, and industry.

By encouraging scientists and engineers to ask "What if?" and "Why not?" our ongoing LDRD investment strategy has reaped long-term rewards for the Laboratory and the nation.

Recent events underscore the contributions of LDRD investments to our evolving national security mission. Most of the counterterrorism technologies fielded by the Laboratory since September 11, 2001 began as LDRD-funded projects. Two examples of long-range LDRD investments that enabled ready-to-go technologies to combat terrorism were the Biological Aerosol Sentry and Information Sys-

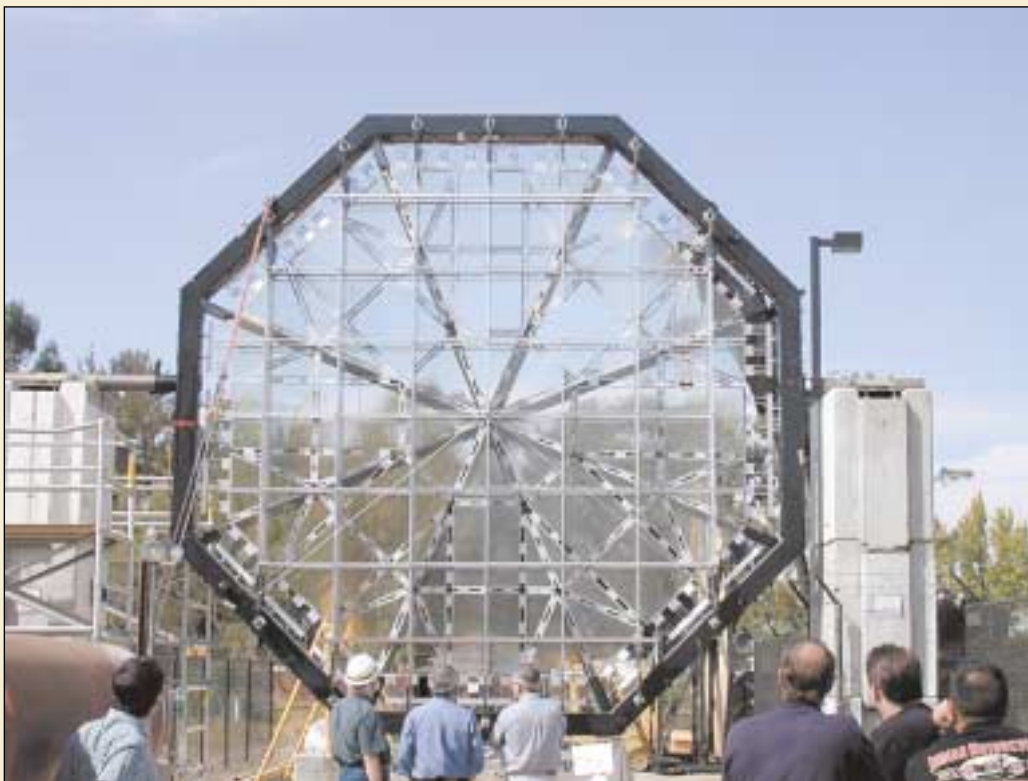
LDRD column, See page 8

Getting 'Up Close' with science

Editor's note: This month's Up Close focuses on Laboratory Directed Research and Development (LDRD) and how it has contributed to Lab missions. Groundbreaking projects are outlined and researchers profiled to show the important role LDRD plays in the innovative science that is the hallmark of this Laboratory.

For information about previous annual reports, see <http://lldr.lnl.gov/ProposalSubmittal/AnnualRpts.html>. ♦

LDRD sparks innovation



The 5-meter Eyeglass diffractive lens is composed of 72 lens panels. Lithographic surface patterning and high-precision assembly make each panel act as a segment of the overall diffractive lens. The result is a lightweight, foldable, high-resolution lens that can be deployed in space for surveillance and scientific uses.

Ralph Waldo Emerson once observed that "invention breeds invention." In essence, that is the idea behind the Laboratory Directed Research and Development Program.

What is Laboratory Directed Research and Development, or "LDRD"? The program provides the Department of Energy (DOE) and the National Nuclear Security Administration (NNSA) laboratories with the flexibility to invest up to six percent of their budget in long-term, high-risk and potentially high-payoff research and development in support of national secu-

Overview, See page 8

The LDRD process

Proposals for Laboratory Directed Research and Development (LDRD) funding undergo a rigorous selection process to guarantee the highest standards of technical excellence and the best fit with the strategic goals of the Laboratory and DOE/NNSA missions. Each of the major LDRD project categories — Strategic Initiative, Exploratory Research, and Laboratory-

Process, See page 8

Cutting-edge research revitalizes plutonium science

The first results from Joe Wong's latest Laboratory Directed Research and Development (LDRD) project are already sitting at *Science* magazine recently accepted for publication in an upcoming issue.

The work — the first full mapping of all of the phonons (the vibrational modes of the crystal lattice) in gallium-stabilized delta-Pu — and future experiments promise to reveal much about the chemistry and thermal properties of plutonium and its alloys. It was performed with Co-Investigators Dan Farber of E&E and Adam Schwartz of CMS and post-doc Florent Occelli of E&E.

The groundbreaking work, which should significantly benefit the Lab's defense mission, is only one of several LDRD projects Farber has been a part of since first coming to the Laboratory as a student in 1990.

Farber began his Lab career as an LDRD-funded student working in the Institute for

Geophysics & Planetary Physics.

"When you're a scientist at the Lab with what you think is a good new idea, theory or technique, LDRD is often really the only avenue for developing that idea," said Farber, a mineral physicist. "We appreciate how important that avenue is to basic science, and how much the benefits accrued feed back into core Lab programs. I can't imagine doing without it."

"The measurement and understanding of the phonon properties of plutonium are very basic science and will help us understand this material's unusual properties" explained Farber, "but equally important, measurements of this type are also critical to programmatic research and will ultimately contribute to building confidence in the performance characteristics of plutonium and its alloys"

The rapid results in the research were possi-

Pu, See page 5

Supercomputing meets future needs

The Computation Directorate has long used Laboratory Directed Research and Development (LDRD) funding to develop new capabilities in anticipation of programmatic needs, especially in the area of large-scale scientific simulation. Two LDRD Strategic Initiatives in the 1990s led the directorate and the Laboratory into the world of massively parallel computing and accelerated the emergence of simulation as a peer to theory and experiment in the process of scientific discovery.

The evolution of “supercomputing” since that time has put the Laboratory at the forefront of scientific computing and has had a profound impact on disciplines across the Lab, from weapons science, physics and chemistry to bioscience and engineering. It also made the Computation Directorate a world leader in computing research.

Eugene Brooks helped pioneer parallel computing by building capabilities in large-scale simulations, thereby enhancing Computation’s core competencies (see accompanying article). Mike McCoy later



Mike McCoy

led an LDRD Strategic Initiative to make newly developed “high end” computing capabilities available to researchers across the Laboratory to do “science of scale.” “I see that as a turning point where we started using high-end computers to enable large-scale science,” said Steven Ashby, deputy associate director for Computing Applications and Research in the Computation Directorate.

Subsequent Computation LDRD investments in scalable numerical algorithms, multi-resolution scientific visualization, and computational science contributed to the successes in projects varying from stockpile stewardship to groundwater remediation. They also have enhanced the Directorate’s standing in the scientific computing community. For example, cutting-edge visualization capabilities developed by Mark Duchaineau and his colleagues earned the high-performance computing field’s most coveted award — a Gordon Bell Prize — in 1999.

More recent LDRD projects helped to position the Computation Directorate for its major role in Scientific Discovery through Advanced Computing (SciDAC), a 5-year program in the DOE Office of Science. This program develops scientific computing software and hardware infrastructure needed to use terascale computers to advance DOE research programs in basic energy sciences, biological and environmental research, fusion energy sciences, and high-energy and nuclear physics.

At present, Computation’s LDRD projects are focused in areas relevant to homeland security. This is particularly true of its Exploratory Research in the Institutes (ERI) data science theme, which is carried out in the Lab’s Institute for Scientific Computing Research (managed by the Computation Directorate for the University Relations Program). These and future LDRD projects are well aligned with the Laboratory’s emerging science and technology longrange plan.

Killer micros change computing

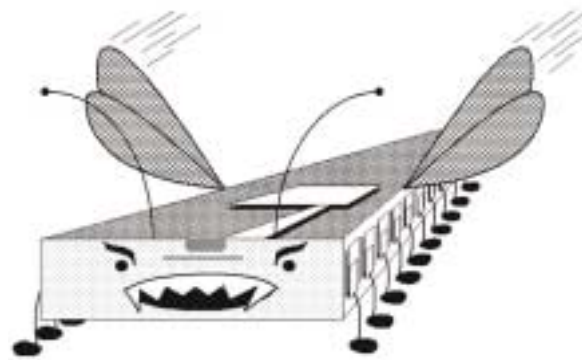
By the early 1980s when the growth in the processing power of mainframe supercomputers had begun to stall, a small group of computer scientists began casting around for new directions.

When Eugene Brooks came to the Laboratory in 1983 from Caltech, the Lab had a modest parallel-processing effort in Computation and Physics “focused on relatively small machines.” Only a few places, such as Caltech, were looking seriously at parallel processing as an alternative to traditional mainframes.

Chuck Leith, who was in A Division at the time, wrote a report recommending Laboratory Directed Research and Development (LDRD) funds be used for a Massively Parallel Computing Initiative, a radical notion in the computing community in the late 1980s.

“We were heretics,” recalls Brooks. “They used to laugh us out of talks.”

Using LDRD funds for the three-year project, Brooks and fellow researchers worked on massively parallel computing systems at the



Lab and remotely on machines at Caltech and other DOE institutions.

They became convinced that the future of high-performance computing lay in many microprocessors working in parallel, not the traditional mainframe technology, which relied on a small number of large, centralized processing units. Brooks dubbed it “the attack of the killer micros.”

“Parallel computing was the only way we were going to get an increase in computer performance,” he said.

That LDRD Strategic Initiative led to the broad use of parallel computing in the weapons program and in energy research, notably at the National Energy Research Supercomputer Center (NERSC). It paved the way for the massively parallel machines that are now a cornerstone of stockpile stewardship’s Advanced Simulations and Computing.

“It was really vital to the start of parallel computing and led to the critical mass that has made supercomputing what it is today at the Lab,” Brooks said.

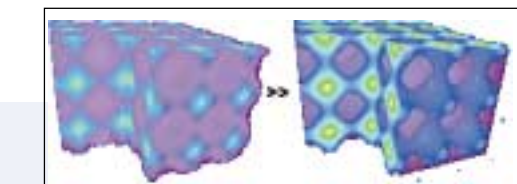
“This was a classic LDRD story,” he added. “More than a decade later, it is still surprising to see how predictive we were.”

Powering up some large-scale visualization

Less than a year into his new job at the Lab, Valerio Pascucci was well on his way to figuring out how large-scale visualization projects could enable interactive data exploration on something smaller than a power wall display.

When he arrived at the Lab in 2000, he worked in close collaboration with an existing visualization Laboratory Directed Research and Development (LDRD) Project in the Computation Directorate. It was there when Pascucci realized that a radical change in software design would allow developing large-scale visualization codes, such as for real-time display of global climate change models, that could run on something as small as a laptop computer.

“Most people didn’t believe this could be done,” said Pascucci, 35. “Scalability was one of the major issues. The question was how could you get a large amount of data on a small screen. Data transfer often takes a long time. But we figured out how to load the most important data on the fly so that good geometric approximations can be visualized almost instantly. Using progressive algorithms allows us to improve automatically the quality of the approximations as the user focuses on a particular region of interest. Now, researchers can



Valerio Pascucci has created a code for real-time monitoring of large scientific simulations through an LDRD project.

Valerio Pascucci

visualize, on their desktop PC, a large-scale simulation while it’s being executed on a remote parallel supercomputer.”

By using a one-way streaming infrastructure, Pascucci and his team developed a code that synchronizes flow in one direction. “Instead of storing the data in a standard matrix format, you can speed up the data access using hierarchical space-filling curves,” he said. “With this new technology we developed a code with the ability to scale throughout the platforms.”

He said LDRD seemed like the logical course to pitch his idea of eliminating the long delay in visualization projects.

“LDRD was a good choice,” he said. “It’s clearly the place where you can do basic research and you can see the impact on the users.”

Pascucci’s Exploratory Research project ends in 2004, and he intends to have at least 15 users by the end of the project.

“We want to cover at least one code in each directorate so we can demonstrate the technology and eventually get the opportunity to continue the R&D work,” he said. “We just need to get the technology out to the users.”

Creating new tools for technology gap in weapons detection

In the fight against terrorism, new tools have been sought for inspecting the millions of cargo containers that enter the United States each year.

One LDRD project aimed at filling this technology gap was started in early 2002 under the direction of Lab nuclear chemist Arden Dougan.

The project looked at a promising approach – using neutrons to detect nuclear and chemical weapons, nuclear materials, chemical warfare agents, and high explosives.

Called “active neutron interrogation,” the approach involves shooting neutrons into the cargo containers and searching for the presence of terrorist materials by the nuclear signatures emitted.

The research has spurred the development of a new radiation detector for field use, said Dougan.

This research has since been transitioned to funding from the NNSA.



New tools have been sought for inspecting the millions of cargo containers that enter the United States each year.

Early biodetection investment paid off

In the weeks after September 11, Livermore researchers speedily moved into the field with two biological detection systems.

They were ready, in large part, because of the Laboratory Directed Research and Development (LDRD) Program, which had invested funds to develop biodetection capabilities, notes physicist Fred Milanovich.

“LDRD was of fundamental importance to our readiness,” Milanovich said. “The process that the government uses normally takes 6 to 18 months for a great idea to end up with funding.

“An organization that doesn’t self-invest will rarely make the state of the art happen. LDRD is about the only way we can self-invest.”

A 32-year Laboratory employee, Milanovich headed the Lab’s Chemical and Biological National Security Program (CBNP) between 1996 and 2002. He is now an Edward Teller Fellow of the Laboratory, whose research is independently supported.

Following the 2001 terrorist attacks, the Laboratory deployed several technologies developed partially with LDRD funding; one was the Biological Aerosol Sentry and Information System (BASIS), which reduces the time to detect pathogens from weeks or days to less than a day. It was developed in conjunction with Los Alamos National Laboratory.

The other system that was rapidly available after September 11 was the Handheld Advanced Nucleic Acid Analyzer (HANAA), a portable, battery-operated instrument that can identify pathogens in the field.

“To CBNP, the LDRD Program was the single most important source of funding in our early days,” Milanovich remembers.

“Don Prosnitz



Fred Milanovich is a physicist whose research is independently supported.

and others here at the Laboratory correctly anticipated that bioterrorism would be more of a threat to the civilian sector than to the military.”

Milanovich recalled he, Ray Mariella and Prosnitz in the mid 1990s put together a white paper of Livermore technologies that could be used to counter terrorism.

The paper drew the support of Wayne Shotts, associate director for Nonproliferation, Arms Control, and International Security (NAI) and others in the NAI directorate, who supported several LDRD proposals.

With the added support, the Lab’s fledgling Chemical and Biological National Security Program attracted support from outside funding agencies.

Today, seven years later, HANAA is available commercially as Bio-Seeq™, from Smiths Detection.

A four-year, \$16 million investment in adapting flow cytometry technology to biodetection has led to the Autonomous Pathogen Detection System, the next generation after BASIS. And, a third-generation system called RAIDDS, short for Rapid Automated Integrated DNA Detection System, is under development by a team led by biomedical engineer Tony Makarewicz and mechanical engineer Ed Schmidt.

These days, the 58-year-old Milanovich is looking out into the future 10 to 20 years to see what will be needed on the horizon for biodefense.

“Detection is a large challenge,” he said. “Currently we are only as safe as how well we plan for what we know. I want to be ready for the unknown.”

Specifically, he is thinking about ways to handle the three “B’s” — bioevolution, bioterror and bioerror.

Handheld Advanced Nucleic Acid Analyzer (HANAA), a portable, battery-operated instrument that can identify pathogens in the field.



University collaborations help push the boundaries of science

For researcher Glen Nakafuji, the Laboratory Directed Research and Development (LDRD) has provided the chance to do one-of-a-kind experiments he wouldn’t otherwise have been able to do.

For example, in the first LDRD project that Nakafuji led, his team studied how chemical warfare agents disperse upon release from an intercepted ballistic missile.

As a part of the experiment, Nakafuji and his team simulated a liquid release from an altitude of 70 kilometers (about 210,000 feet) at the Alpha Pulsed Supersonic Wind Tunnel at UC Santa Barbara. Previously, almost all simulated liquid release experiments had been conducted at

sea level.

“People thought that with increased aerodynamic force on a liquid, certain break-up patterns could be expected,” Nakafuji said. “But the expected break-up patterns were not accurate.”

In effect, Nakafuji’s team showed that previous research in the field was wrong and helped develop a better understanding of the dispersal of chemical warfare agents from intercepted missiles or missiles that function normally by releasing agents at a preset altitude.

In addition to helping him conduct unique experiments, LDRD has exposed Nakafuji to more work with multidisciplinary teams and helped push the bound-

aries of computational modeling, he said.

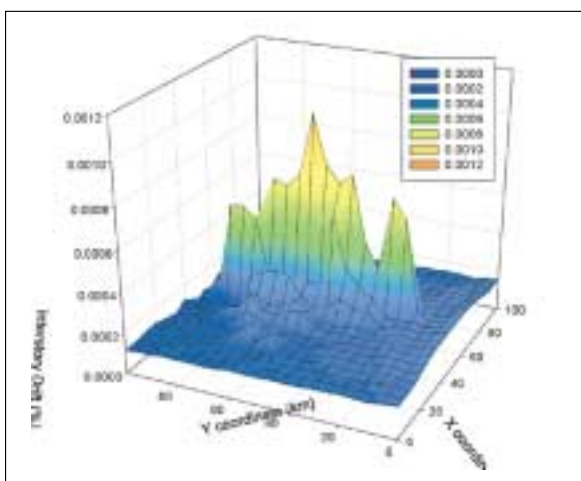
A physicist in the Proliferation Detection and Defense Systems Program (Q Division), the 35-year-old Nakafuji has worked at the Laboratory for five years. Previously, he worked for five years at Los Alamos National Laboratory.

In a new LDRD project this year, Nakafuji and a small team of physicists and engineers are examining how to identify what type of weapon of mass destruction material might be on an intercepted missile.

Information from such detection would allow battlefield commanders and other decision-makers to take appropriate responses (e.g., protective action for troops).

Simulating ground, building response

Working in conjunction with the Defense and Nuclear Technologies Directorate, Engineering's Principal Investigator Dave McCallen and Energy and Environment's Shawn Larsen with their team of earth scientists and engineers have developed a simulation model for regional ground motions and building response in Southern Nevada. The six-billion-zone model extends from north of the Nevada Test Site (NTS) south to cover the Las Vegas basin. This model is being used to estimate the ground motion hazard in the Las Vegas Valley



A building in the Las Vegas Valley responds to a strong ground motion from a large earthquake in this spatial display of structure demands

ing the infrastructure risks to Las Vegas and the surrounding communities. The team will also evaluate the response of post-1992 modern high-rise structures to a blast of at least 150 kilotons.

if nuclear tests resumed at the NTS.

The two-year study began in February 2002, and the model is now being used to simulate underground explosions at the NTS, propagation of seismic waves from the NTS to the Las Vegas Valley, and the dynamic response of buildings in Las Vegas for the predicted ground motions. Because Las Vegas has changed significantly since 1992, the time of the last underground test, the team's programmatically funded work will now focus on defin-

Seed money for disposable pathogen detection

When Elizabeth Wheeler attended Livermore High School more than a decade ago, she never thought she'd wind up working at the Laboratory.

Though she always had an interest in math and science, working at the Laboratory wasn't necessarily her ideal career at that point in her life.

"I never dreamt that I'd come back here and work at the Lab," the 31-year old chemical engineer said. "In high school, I always made fun of those Lab workers biking around with their badges on. Now I'm one of them."

With a chemical engineering degree from UC Davis and a Ph.D. in chemical engineering from Stanford University, working at the Laboratory turned out to be a great move, she said.

As the Principal Investigator for the Exploratory



Jacqueline McBride/Newsline

Elizabeth Wheeler is working on a disposable device that can detect biological agents.

directorate before going to the LDRD committee," she said. "LDRD is good because it's seed money for a project. It's a good way to work on more fundamental science."

The disposable PCR device is a pathogen detection tool that eventually will run off a battery and is inexpensive enough that it could be thrown away after each use.

Research Laboratory Directed Research and Development (LDRD) "Disposable Polymerase Chain Reaction Device," Wheeler said she somewhat redefined the three-year project back in December 2000 when she had to represent it to the LDRD committee.

"The nice thing about the Exploratory Research projects is that you have a sounding board through the

A mini source for mighty power

With just a few months left of their Laboratory Directed Research and Development (LDRD) funding, members of a team working on a microfluidic fuel processor for miniature power sources say they are pleased with the results of their effort.

"Our original goal was to develop a 500-milliwatt fuel cell," says

Principal Investigator Ravi Upadhye. "We have exceeded our

objectives by more

than a factor of ten. We are very happy with the way this project has gone."

The project team has sought to develop a lightweight, reliable power source for reconnaissance and intelligence-gathering sensors and for telemetry applications. The thin-film fuel-cell power source can also provide portable electrical power for a range of consumer electronics such as cellphones and laptops. A fuel cell module, consisting of a microreactor for generating hydrogen, is expected to provide portable electronics with operating times three times longer than current rechargeable batteries.

"A cellphone needs about 5 watts, and we can get to about 6 watts with our fuel cell," said Upadhye, who was a member of Engineering's New Technologies Engineering Division when the project started three years ago; today Upadhye is the deputy Materials Program leader for the Energy and Environment Directorate in Chemistry and Materials Science. "A laptop needs about 10 watts and we hope to reach that in the near future."

Upadhye said the LDRD funding for the past three years made it possible for the team of Engineering and CMS personnel to complete a prototype of the technology.

Co-Investigator Jeff Morse of Engineering's Electronics Engineering Technology Division said a Commercial Research and Development Agreement (CRADA) is in place with a commercial partner, who has licensed the technology. "We expect continued support of this work to follow for homeland security applications," added Morse.



The thin-film fuel cell.

Vision led to early bioweapon detection work

Ray Mariella Jr., director of Engineering's Center for Micro and Nano Technology, describes himself simply as a "technical person" who loves challenges.

Mariella says he enjoys working at a lab that "enables and values teamwork," adding "This Laboratory values competency in a way I have never seen elsewhere."

Today, Mariella is leading an interdisciplinary team on an LDRD-funded project titled "Nanoscale, Deterministic Fabrication of Mesoscale Objectives."

Entering its third year in FY04, the project seeks to provide a better understanding of the chemical and physical processes that influence materials that are exposed to femtosecond laser pulses. The work has applications to the Lab's Stockpile Stewardship Program, the National Ignition Facility (NIF), and Defense & Nuclear Technologies (DNT) high-energy-density science research.

Mariella says one of his significant accomplish-

ments occurred in the 1990s, when he wrote the Lab's first counter-bioweapons (BW) instrumentation proposal. Research growing from that proposal provided some of the technical groundwork that served to help the Laboratory secure an early role in the DOE's chemical- and biological-weapons detection program.

At the time a member of the Biology and Biotechnology Research Program, Mariella was asked by Donald Prosnitz, a division leader in Nonproliferation, Arms Control, and International Security (NAI) to write the original LDRD Director's Initiative to develop a portable BW detection system. "Don had the vision to redirect my work from genomics to counter-bioweapons," says Mariella.

The portable BW detection system combined two relatively new Lab inventions, both of which Mariella had a role in developing: a miniature flow cytometer and a polymerase chain reaction instrument, the forerunner of today's Handheld Advanced Nucleic-Acid Analyzer (HANAA) (see page 4).

Investigating properties of dense hydrogen

Sam Weir completed his post-doc work with Lab physicist Bill Nellis in Physics' H-Division after graduating from Cornell in 1989.

He spent three years with Nellis, and then was hired as a B-Division staff scientist. When a team led by Nellis received Laboratory Directed Research and Development (LDRD) funds in 1993 to investigate the properties of dense hydrogen in the "near metallic" regime — pressure in excess of a million times the Earth's atmospheric pressure — Weir returned to work with Nellis part-time on the project.

Understanding the behavior of the simplest and most abundant element in the universe had implications for Stockpile Stewardship weapons science, inertial-confinement fusion studies planned for the National Ignition Facility (NIF), and the study of the planet Jupiter.

Using the two-stage gas gun, the team succeeded in compressing liquid hydrogen into a metallized state, a long-standing challenge of the high-pressure-physics community.

"It was a really good experience for me," said Weir, adding it gave him valuable background in shock-wave physics that has served him well.

Weir, who has since moved to Defense & Nuclear Technologies (DNT), is now working in static high-pressure experiments and is completing work on another groundbreaking LDRD project.

Working with the Lab's Damon Jackson, Reed



From left: Art Mitchell, Sam Weir and Bill Nellis stand near the two-stage gas gun.

Patterson, Vince Malba, Chantel Aracne-Ruddle, and Dave Ruddle, Weir is bringing the newest capabilities to high pressure studies by developing advanced, new diagnostics for high-pressure experiments. This is a capability "unique to the Laboratory," he said.

The team is developing "designer" diamond anvils. This technology allows electrical circuitry to be designed and emplaced inside the diamond tip of the anvil to produce finely controlled magnetic and electric fields, enabling a new level of capability and control in high-pressure measurements.

Understanding how pathogens cause illness

Improved detection systems and help for developing vaccines and drugs could come from a major Laboratory Directed Research and Development (LDRD) research initiative in the homeland security area.

Now in the last year of a three-year effort, the Pathogen Pathway Project is examining what makes pathogens virulent and able to overcome the biological defenses of a host organism.

The project is studying several bacteria that have very similar DNA sequences (over 90 percent identical) but that cause dramatically different symptoms in people, some producing only a cough or diarrhea and others causing deadly pneumonic and bubonic plague.

"We're looking at the differences in DNA and in symptoms as clues to what the pathogens use to make people sick," said project leader Pat Fitch, who also heads the Chemical and Biological National Security Program.

About a dozen biologists, chemists and computer scientists are attempting to identify and characterize the genes and proteins involved in virulence and in the response of the host organism.

"We're pushing hard to see how much of this work can be done using computers," Fitch said. "We're using the computers to analyze the data, and we're using them to predict the outcome of the experiments, or to augment the experiments."

As a part of the project, one of the pathogens that has been studied is *Yersinia pestis*, the causative

DNT develops new versatile science tools

Recent Defense & Nuclear Technologies (DNT) projects have included several themes:

- Leading-edge work in developing new techniques in high-pressure physics. Among these are developments of new types of diamond anvil cells and other experimental platforms and techniques for high-pressure measurements. Examples include the designer diamond anvil cell, the development of techniques for measuring equation of state on pulse-power machines such as Sandia's Z machine, and the development of Nova- and Omega-based techniques for studying the properties of materials at ultra-high strain rates. The last two techniques can be transferred to the National Ignition Facility (NIF).

- Development of techniques to measure the atomic and microscopic origins of material strength and failure, to enable a predictive capability of material response to be developed. Projects in this area include studying rapid resolidification and material failure at various strain rates. The development of techniques to understand matter at elevated temperature is an area funded recently. Computational techniques for collisional plasma physics and experimental studies of warm, dense matter were projects of this type.

- Development of new imaging techniques, such as proton radiography and femtosecond diagnostic techniques, that reveal more information about microscopic processes.

agent of plague.

The project researchers have also performed fast-turnaround studies in support of federal and state agencies in the development of better detection assays for West Nile disease and foot-and-mouth disease.

PU

Continued from Page 1

ble because of earlier studies of iron and cobalt under very high pressure, supported by Institute of Geophysics and Planetary Physics LDRD funding, and conducted by Farber and other colleagues at the European Synchrotron Radiation Facility in France. The research techniques learned at the ESRF laid the groundwork for the plutonium discoveries at this same facility.

At the same time as these early studies on iron and cobalt, the LDRD program was helping to revitalize plutonium research at the Laboratory and contributed significantly to National Nuclear Security Administration's program to ensure the safety and reliability of the nation's aging nuclear deterrent without testing — the Stockpile Stewardship Program.

Scientists have long been fascinated by plutonium's (Pu) unique characteristics and changeable properties. Pu reacts vigorously with its environment, particularly oxygen, hydrogen and water, thereby degrading its properties from the surface to the interior over time. In addition, Pu's continuous radioactive decay causes self-irradiation damage that can fundamentally change its properties over time.



Jacqueline McBride/Newsline

From left: Chantel Aracne, Carl Boro, Florent Occelli and Daniel Farber.

The LDRD investments in Pu science helped generate the capability to overcome many of the difficulties and prepare high quality Pu samples for these demanding experiments.

"Seemingly unrelated work turned out to be exactly what was needed for this plutonium project," Farber said. "When you make investments in good quality, fundamental science, the unexpected payoffs can be great."

An earlier LDRD, led by Michael Fluss, determined the temperatures at which lattice defects in Pu alloys begin to migrate. This work provided much needed data to the Enhanced

Surveillance Campaign, which is interested in how the self-irradiation damage of Pu may lead to changes in properties as the Pu ages.

Fluss designed and constructed a specialized experimental resistivity chamber that is currently being used to evaluate the fundamentals of the d-a' phase transformation in Pu alloys that results in a large, 20 percent volume contraction. Principal Investigator Adam Schwartz said: "This project combines experimental characterization such as advanced transmission electron microscopy to evaluate nanometer-sized defects, and electrical resistivity and differential scanning calorimetry to track the changeable properties with phase field and finite element modeling to elucidate the crystal geometry, particle shape, and speed at which the transformation proceeds of this important and intriguing phase transformation."

In addition, it has resulted in the hiring of a post doc and two term employees to the Laboratory." There are two additional Pu-science-based LDRDs currently on going. One, led by Patrick Allen, focuses on the thermodynamics of Pu, extending the ability to calculate binary and ternary phase diagrams and the second, led by Alex Hamza, is attempting to experimentally benchmark current and future electronic structure models.

Bioengineering projects range from microbes to cancer research

Harnessing the power of microbes

Life as we know it would be impossible without the work of microbes. The oldest and most diverse form of life on Earth, microbes inhabit and influence nearly every environment and can thrive under extreme conditions of heat, cold, acidity, pressure, and radiation. By studying their molecular processes in an Laboratory Directed Research and Development (LDRD) funded project led by Michael Thelen of Biology & Biotechnology Research Program (BBRP), LLNL scientists hope to discover the biochemical mechanisms by which certain microbes alter toxic metals and radioactive substances like uranium. The research could lead to new ways to use the microscopic creatures to help clean up toxic and radioactive waste sites.



Determining how genes are regulated

Now that the DNA sequence of the human genome has been determined, the next big step in human biology is understanding the complex mechanisms that regulate when and where particular genes are turned on and off, or “expressed,” in different types of cells and under different environmental conditions. LDRD has funded an LLNL team led by Krzysztof Fidelis of BBRP to develop computational tools to analyze these regulatory mechanisms and generate mathematical models of gene expression. The team will build on LLNL’s work in identifying gene functions in human chromosome 19 and in comparable areas of the mouse genome.

Peregrine: Better way to target cancer cells

One of LLNL’s most successful LDRD projects in the biosciences is Peregrine, an advanced method for targeting tumors with radiation treatment. Peregrine allows doctors to direct radiation at tumors, while minimizing damage to surrounding healthy tissue, by precisely determining the dose of therapeutic radiation in the body. Development at the Laboratory began in 1994 by an LDRD-funded team led by Christine Hartmann-Siantar, the technology was licensed to NOMOS corporation in 1999, and is being distributed to hospitals and clinics nationwide.

Allen Christian: A problem solver

He says it suits his “short attention span,” but the number of research projects that molecular biologist Allen Christian has worked on over the past five years could easily fill the career of a more specialized researcher. Since arriving at LLNL in 1998, Christian and his bioengineering team in the Biology & Biotechnology Research Program’s Defense Division have taken on a wide variety of special projects, with enviable results.

So far the team’s “Renaissance” approach to basic research has garnered it two R&D 100 awards — for a technology that can efficiently locate damaged DNA within a cell, and another technique that can quickly find and determine the function of genes — as well as one granted patent and eight more patents pending.

Christian’s team has two current Laboratory Directed Research and Development (LDRD) funded projects. In one project, the team is developing a method of “silencing,” or turning off, genes using exotic molecules called “siHybrid” — small, double-stranded molecules consisting of one strand of DNA and one of RNA (ribonucleic acid, a molecule that helps produce proteins) that can be dropped on any cell and can be used to shut down any gene. The molecules are being tested against the HIV virus and



Developers of the award-winning Gene Recovery Microdissection process are (left to right) Matthew Coleman, Allen Christian and James Tucker.

S&TR

prostate-cancer-causing genes, both with preliminary success.

In the other project, the team is developing a technique for making precise, quantitative measurements of the processes occurring in individual cells. The goal is to obtain numerical data that will allow predictive computational modeling of cellular processes — a capability that would be especially useful for developing new pharmaceuticals.

Fusion of efforts creates new discipline

Mike Colvin feels very fortunate to have had Laboratory Directed Research and Development (LDRD) support for two major endeavors he has been involved in creating: the Computational and Systems Biology capability in the Biology & Biotechnology Research Program (BBRP) and the Physical Biosciences Institute (PBI).

“Many of the people and projects are here thanks to an LDRD Strategic Initiative (SI) in computational biology,” says Colvin, CSB division leader. “Indeed, two group leaders, Felice Lightstone and Daniel Barsky, were originally hired as post-docs for that project, as was Eric Schweidler (now a staff physicist in H-Division).”

Colvin said the SI’s goal has been to build a Lab capability in computational biology that applies Laboratory expertise in advanced simulations and supercomputing to perform accurate molecular simulations of biochemical processes.

“The main focus of our biological modeling has been the structure and consequences of DNA damage, which ties in well with many of the experimental biology projects in the BBRP,” said Colvin. This theme has included simulations of DNA repair and replication enzymes, DNA-binding anticancer drugs, and DNA-mutating chemicals formed in some foods during cooking.

“Thanks to the LDRD support we have been able to publish dozens of articles in computational biology, which has been critical to our successes in getting outside funding to continue our biological modeling projects,” he said. With the project in its final year, researchers are “busily writ-

ing up the final research results and submitting grant proposals to external funding agencies.”

LDRD funding, said Colvin, “is absolutely essential” to creating new scientific programs at the Laboratory. The computational biology program, he said, is “a great example” of how LDRD “can prime the pump” for external funding.

“Funding is so competitive that you really need to have a very solid track record in the specific area for which you are applying for funding,” said Colvin. “You can’t typically get a grant for just an idea or concept. You need to have papers published that demonstrate your concept will work.”

Said Colvin: “LDRD allowed us to get the publications and, through giving talks at conferences and universities, the recognition so that we can be competitive in this area. To this end we have been pretty successful.”

Many of the computational biology projects that were originally started under this LDRD are now funded by external grants. One example is continuation of work on food mutagens that is funded by the National Institutes of Health.

LDRD funding, Colvin explained, has been central to the newly formed PBI.

“Without LDRD support, the PBI concept would not be possible at LLNL,” said Colvin.

PBI creates an incubator for multidisciplinary post-doctoral projects that link LLNL experimental and simulation capabilities to research projects in quantitative biology. It also seeks to attract and train future talent for LLNL life sciences.

A new model for climate change study

When Starley Thompson stood before the Laboratory Directed Research and Development (LDRD) committee in 1999, he approached the members with a proposal in climate modeling that had never before been attempted.

As an expert in climate and earth science, Thompson came to the Lab to work on climate research, which soon led him to start an LDRD Strategic Initiative.

This was an unprecedented proposed project to couple atmosphere-ocean climate, terrestrial biosphere and ocean-carbon cycle models to more realistically predict future climate change and the increase of carbon dioxide.

"We proposed development and testing of a model in an area where people hadn't put these models together before," Thompson said. "We have developed the highest resolution, fully coupled model. We are at the forefront of this kind of modeling."

The goal of the INtegrated Climate and Carbon (INCCA) SI is to develop a comprehensive coupled carbon/climate simulation model that can both predict future climate change and have an emphasis on defining, bounding and reducing the uncertainties that are



JACQUELINE MCBRIDE/NEWSLINE

Starley Thompson is working on a carbon/climate simulation project that can predict future climate change.

important to policymakers.

The models run over a 230-year cycle, beginning in 1870, which serves as a pre-industrial period, out into the future to the year 2100. Thompson said early data on carbon dioxide concentrations is not as hard to come by as most would think. By looking at the air bubbles trapped in ice cores, Thompson's team can observe the carbon dioxide concentration at any given time. And beginning in the 1950s, there are detailed records of atmospheric carbon dioxide.

"We have a pretty good idea of carbon emissions by looking at records of how much fossil fuel has been burned over time," he said. "We use projections of carbon emissions to run our model into the future."

"We decided we'd put this LDRD SI together because the Department of Energy is the agency most directly involved with carbon," he said. "This serves DOE's interests."

In its third year, the \$3 million project has achieved most of its goals: to accurately model the carbon emissions from 1870 to 2100 by comparing the results to actual observations over that same time frame.

Thompson said LDRD is a great option for funding projects that at first glance, may to appear out of the box.

"It's a tax that supports the people who have ideas that may pan out in the future. It does help get some projects off the ground."

Water initiative teams disciplines

The Energy and Environment Directorate has moved in a new direction when it comes to Laboratory Directed Research and Development (LDRD) projects. Beginning this year, the push has been toward multidisciplinary teams looking to help solve some of the issues related to one precious resource: water.

The Water Initiative consists of three LDRD proposals.

One of the projects within the initiative will use regional climate models created at a scale of 20 to 30 kilometers to address the effects of climate change and variability on the supply and demand for fresh water in the coming decades. Principal Investigator Philip Duffy will demonstrate the use of his model to assess the extent to which California is vulnerable to climate change and how water availability is critical to its survival. Ultimately, the projections will help regional and state water officials assess the possible need for change in water management practices.

Another project within the Water Initiative could have worldwide impacts on water availability. Principal Investigators Kevin O'Brien of the Engineering Directorate and Bill Bourcier of the E&E Directorate are working on a water-purification process using molecular engineering to create new types of electrodialysis membranes.

The third piece of the Water Initiative addresses the need for more effective management of water quality in groundwater basins. The research effort, led by Principal Investigator Brad Esser of Chemistry & Materials Science and involving researchers from the E&E Directorate and the Environmental Protection Department, focuses on nitrate contamination in groundwater.

Researching the mysteries of particle physics

Doug Wright's introduction to Laboratory Directed Research and Development (LDRD) came in 1993, as a post-doc, fresh out of Princeton. He came west to work on LLNL's collaborative research work on the Superconducting Super Collider, being built in Texas.

But just a month after he joined the Lab, Congress cancelled the \$8.3 billion collider project, and Wright was out of an assignment.

His involvement with LDRD has proven much more successful.

Working with other Lab scientists, Wright has been researching a long-standing mystery of particle physics: the mismatch of matter versus antimatter in the universe. The



Doug Wright does particle research at the Stanford Linear Accelerator Center.

group, which Wright heads, has been instrumental in analyzing the decay of subatomic B mesons collected at the Stanford Linear Accelerator Center.

Wright gives major credit to LDRD. "LDRD was crucial for us to get involved in the project," he said. "LDRD is essential to the Lab and serves three very important functions. First, it keeps us at the forefront of these revolutionary basic science experiments. Second, it helps attract high-caliber, early-career academics who would otherwise perceive LLNL as just a weapons lab. And finally, it builds up capabilities that can have important programmatic benefits."

New nuclear fuel is in the STARs

Development of a new nuclear fuel is the subject of a first-year Laboratory Directed Research and Development (LDRD) project, entitled Mono-Nitride Fuel Development for STAR and Space Applications. The project seeks to advance development of a uranium nitride fuel for use in a STAR (Small, Transportable, Autonomous Reactor) nuclear reactor. The STAR features a sealed reactor vessel that can be shipped to a user and returned to the supplier without ever having been opened in its 30-year operating lifetime. This would reduce the possibility of weapons proliferation issues.

Broadening science base for Lab missions

What is today the Laboratory Directed Research and Development (LDRD) Program began at the Laboratory in the early 1980s as Institutional Research and Development (IR&D) under the direction of former Director Michael May.

The program to provide federal laboratories with discretionary funds for scientific research and development resulted from a recommendation of a blue ribbon panel chaired by David Packard, chairman of Hewlett Packard and a former deputy secretary of Defense.

Appointed by the White House in 1983, the “Packard Panel,” as it came to be known, was charged with coming up with ways to improve the use and performance of the federal government’s 700 research laboratories, including those operated by contractors, like LLNL and other UC-managed facilities.

Roger Batzel, then Lab director, appointed May to start up and run the IR&D program. May put together a review board made up of well-respected scientists and engineers that cut across Lab programs. Among those who served on the board was John Nuckolls — “a great one for innovation,” said May — who would succeed Batzel as Lab director.

May said the Packard Panel concluded

that some important areas of research related to laboratory missions were possibly being overlooked because these areas were outside the scope defined by Congress.

“The idea was not to go into the wild blue yonder, but to broaden the Laboratory’s security and energy missions and their underlying science,” May said, adding that it was better for the programs “not to be totally bound by bureaucratic restrictions.”

There was recognition of a need to “stimulate new ideas that could be used in major programs,” he said, “and a valid concern about where new ideas and directions come from. You need several routes



Michael May

for funding ideas, otherwise people just keep doing what they have been doing.”

The IR&D Program was a way for initiatives recognized as good ideas, but which didn’t fit neatly into a program, “to find a niche,” said May.

Funding was made available in several different categories: Lab-wide, Individual Programs, and a small pot for distribution by the Lab director.

The IR&D Program started as a 2 percent tax on programs. In the early years, some program leaders complained about the tax on programs that IR&D represented, but those dissipated as people came to recognize the value of the program, according to May. On the other hand, he said, “scientists latched onto it eagerly.”

In 1991, Congress established the LDRD Program, providing DOE and NNSA laboratories with the flexibility to invest up to 6 percent of their budget on innovative research (*see accompanying overview article*).

LDRD and its predecessor, IR&D, “have played a major role in keeping up interest and stimulating innovation at the Laboratory,” May said.

Number of LDRD patents as compared to all patents granted to LLNL:						
	1996	1997	1998	1999	2000	2001
Total LLNL patents	83	64	78	84	93	89
LDRD patents	35	29	39	45	35	42
LDRD patents as percentage of total	42	45	50	54	38	47

While LDRD is only six percent of the Lab budget, it is responsible for a disproportionately large percentage of Lab publications and awards. For example, more than 25 percent of Lab publications and 40 percent of R&D 100 awards and patents are attributable to LDRD-funded projects. Moreover, LDRD supports a very large percentage of Lab post-docs, students and university collaborations.

LDRD column

Continued from Page 1

tem (BASIS), which reduces the time to detect pathogens to less than a day, and the Handheld Advanced Nucleic Acid Analyzer (HANAA), a portable, battery operated instrument that can identify pathogens in the field.

In FY03, the LDRD budget of \$65 million sponsors more than 200 projects representing the gamut of research at the Laboratory. Projects are selected through an extensive review process to ensure the highest scientific quality and mission relevance. Each year, the number of deserving proposals far exceeds the funding

available, making the selection a very challenging task.

Despite the rigor of the LDRD selection process, we believe it’s important to be agile enough to respond quickly to new ideas that arise throughout the year. In the Lab-wide Employee Survey conducted in 2001, employees suggested more flexibility in the R&D funding process. In response to this request, the LDRD Program has made more funding available for pursuing small-scale innovative ideas outside the normal review cycle. LDRD funding is available for Feasibility Studies — an LDRD project category for small projects (\$75,000 or less and a maximum of a year in duration) that explore new ideas or challenge

traditional methods.

The LDRD Program is truly a success story. Our projects continue to win national recognition for excellence through prestigious awards, papers published in peer-reviewed journals, and patents granted. LDRD-sponsored projects often lead to technologies that are commercially licensed so that their benefits become available to the nation.

By keeping the Laboratory at the forefront of science and technology, the LDRD Program enables us to meet the challenges of our evolving national-security missions. LDRD nurtures the science and technology that form the foundation of the Laboratory and helps attract the future generations of scientists and engineers.

Overview

Continued from Page 1

ity and other Laboratory missions.

The DOE order creating the program states the objectives of LDRD are to: “maintain the scientific and technical vitality of the laboratories; enhance the laboratories’ ability to address future DOE missions; foster creativity and stimulate exploration of forefront science and technology; serve as a proving ground for new research and support potentially high-value research and development.”

“Since its inception, the LDRD program has played a vital role in supporting the Lab’s core missions,” Director Michael Anastasio said. “In recent years, the program has helped the Laboratory to quickly adapt to new and emerging national-security threats such as bioterrorism.”

LDRD also plays an important role in attracting and retaining the best minds in science and technology. The possibility of receiving funding to pursue individual ideas is a powerful draw for young researchers beginning their R&D careers as well as for veterans who have developed innovative ideas in the course of their Lab careers. In addition, LDRD enables collaborations with industry and academia.

LDRD projects have made important contributions to such Lab mission areas as stockpile stewardship; nonproliferation and counter-proliferation of weapons of mass destruction, including biological, chemical and nuclear; information

Process

Continued from Page 1

Wide— has its own proposal-submittal-and review-process.

For the coming fiscal year, which starts October 1, the process began in February, with the Director’s call for proposals, and ends in August. Proposals for projects in the Feasibility Study category can be submitted throughout the year and are reviewed by the LDRD Office on a case-by-case basis.

LDRD proposal-review committees, composed of senior managers, program leaders, scientists and engineers, and outside experts, review hundreds of

innovative proposals submitted by researchers from across the Laboratory. At the conclusion of the review process in each category, the LDRD Office forwards its recommendations to Laboratory Director Michael Anastasio and his deputy for Science and Technology, who makes the final decision.

Before the beginning of the fiscal year, the LDRD Program submits a one-page summary of each project in its portfolio to the DOE/NNSA for review and concurrence.

For more information on how LDRD projects are selected, contact LSTO (3-2810) or see the LDRD Website: <http://ldrd.llnl.gov/ProposalSubmittal/>.

technology and high-performance computing, as well as environmental research and waste management programs.

Other Lab mission areas supported by LDRD include energy security, environmental stewardship, healthcare technology and breakthroughs in fundamental science and technology.

“The ability to invest in innovative uses of core Lab competencies has spawned new research thrusts such as medical technologies,” said Rokaya Al-Ayat. “LDRD has been instrumental in finding new applications and creating new disciplines for Lab technologies.”

provides the flexibility to explore the feasibility of new concepts. Funded throughout the year, this category allows greater responsiveness to scientists and engineers. Principal Investigators submit proposals through their directorate or directly to the LDRD office rather than to a review committee.

“LDRD has given a new dimension to the concept of multidisciplinary team science pioneered by Lab co-founder E.O. Lawrence,” Al-Ayat said. “LDRD helps foster the creativity, visionary sense of possibility and invention that are hallmarks of this Laboratory.”

LDRD projects are divided into four basic categories:

- Strategic Initiatives focus on innovative R&D activities that are likely to set new directions for existing programs and/or help create new program areas. Projects in this category are generally larger and more technically challenging than projects in other categories. These projects must be aligned with the Laboratory’s strategic plan for science and technology.
- Exploratory Research is aligned with the strategic R&D needs of a Lab directorate or institute.
- Laboratory-wide Competition projects emphasize innovative research concepts and ideas from individual researchers and undergo limited management filtering.
- Feasibility Study/Project Definition is a special category that provides the flexibility to explore the feasibility of new concepts. Funded throughout the year, this category allows greater responsiveness to scientists and engineers. Principal Investigators submit proposals through their directorate or directly to the LDRD office rather than to a review committee.